REPORT

DETERMINATION OF THE AUTO-IGNITION TEMPERATURE (LIQUIDS) OF

[redacted]

NOTOX Project 338636
NOTOX Substance 111834/C

CONFIDENTIALITY STATEMENT

This report contains the unpublished results of research sponsored by [redacted] Chemicals B.V. Reproduction, issue or disclosure to third parties in any form is not permitted without prior written authorisation from the sponsor.

STATEMENT OF GLP COMPLIANCE

NOTOX B.V., 's-Hertogenbosch, The Netherlands

The study described in this report has been correctly reported and was conducted in compliance with the most recent edition of:

The OECD Principles of Good Laboratory Practice

which are essentially in conformity with:

The United States Food and Drug Administration. Title 21 Code of Federal Regulations Part 58.

The United States Environmental Protection Agency (FIFRA). Title 40 Code of Federal Regulations Part 160.

The United States Environmental Protection Agency (TSCA). Title 40 Code of Federal Regulations Part 792.

Study Director

[redacted]

Date: May 03, 2002.

Management

[redacted]

Section Head Analytical & Physical Chemistry

Date: May 13, 2002

QUALITY ASSURANCE STATEMENT

NOTOX B.V., 's-Hertogenbosch, The Netherlands

This report was audited by the NOTOX Quality Assurance Unit to ensure that the methods and results accurately reflect the raw data.

The dates of Quality Assurance inspections and audits are given below.
During the on-site inspections procedures applicable to this type of study were inspected.

DATES OF QAU INSPECTIONS/AUDITS	REPORTING DATES
on-site inspection (s)	
18-Feb-2002 to 01-Mar-2002 (process physical chemistry)	04-Mar-2002
protocol inspection (s)	
13-Feb-2002 (study)	13-Feb-2002
report audit (s)	
16-Apr-2002 (study)	16-Apr-2002

Head of Quality Assurance
[redacted]

Date: 14-5-02

SUMMARY

The determination of the auto-ignition temperature of [redacted]ure (liquids and gases, 1992)",
DIN 51794 "Bestimmung der Zündtemperatur" (1978) and IEC standard 79-4: Method of test for ignition temperature (1975).

Test substance was injected into a test vessel at a temperature range between 20°C and 246°C. The test was performed in triplicate.
A lowest auto-ignition temperature of 214°C was found, with an injection volume of 125 µl.

In conclusion, [redacted] is auto-ignitable with an auto-ignition temperature of 210°C.

PREFACE

Sponsor	[redacted]
Study Monitor	[redacted] ory Affairs
Testing Facility	NOTOX B.V. Hambakenwetering 7 5231 DD 's-Hertogenbosch The Netherlands
Study Director	[redacted]
Study Plan	Start : 13 March 2002 Completed : 13 March 2002

TEST SUBSTANCE

Identification	[redacted]
Chemical name	[redacted]
Description	Clear colourless liquid
Batch	1510-14
Purity	See Certificate of Analysis
Test substance storage	In refrigerator in the dark
Stability under storage conditions	Stable
Expiry date	01 January 2003

The sponsor is responsible for all test substance data unless determined by NOTOX.

Note: **Don't heat up the test substance above 50°C**

With the exception of a small amount for the benefit of the study.

PURPOSE

The determination of the degree of auto-ignitability in terms of the auto-ignition temperature.

GUIDELINES

The study procedure described in this report is based on the following guidelines:

European Economic Community (EEC), EEC-Directive 92/69 EEC, Part A, Methods for the determination of physico-chemical properties, A.15 "Auto-Ignition temperature (liquids and gases)", EEC Publication No. L383, December 1992.

DIN 51794 "Bestimmung der Zündtemperatur", January 1978.

IEC standard 79-4 "Electrical apparatus for explosive gas atmospheres, Part 4, Method of test for ignition temperature", 1975.

ARCHIVING

NOTOX B.V. will archive the following data for at least 10 years:
protocol, report, test substance reference sample and raw data. Thereafter, no data will be withdrawn without the sponsor's written consent.

TEST SYSTEM AND RATIONALE

Apparatus	Self-ignition test apparatus (Sommer und Runge; Berlin, FRG) in accordance with DIN 51794 and IEC standard 79-4.
Rationale	Recognized by the international guidelines as recommended test system (EEC, DIN, IEC).

CALIBRATION OF THE TEST SYSTEM

The test procedure as outlined in this report is validated periodically, using n-heptane (zur analyse; Merck, FRG). The results are in accordance with the criteria of DIN 51794 and IEC 79-4.

PERFORMANCE OF THE TEST

Test procedure

Samples were injected by means of a variable volumetric pipette to assure a rapid injection.
The time lag between injection and ignition was measured for all tests.
Approximately 5 minutes after each test substance injection, the test vessel was flushed completely with clean air (AGA, Amsterdam, The Netherlands).
After flushing, a sufficient time interval was allowed to ensure that the flask temperature was stabilized at the desired test temperature before the next sample was injected.

Preliminary test

For safety reasons (SADT of [redacted] is 50°C), the preliminary test was started at room temperature. Starting at 20°C, every 20°C, 70 µl test substance was pipetted into the test vessel.The temperature rise was about 5°C/min.
Going down from 246°C, the auto-ignition temperature was determined in temperature steps of 5°C using the same injection volume.

Main study

The auto-ignition temperature was determined going down in steps of 2°C. In the first test, 30, 70 and 150 µl test substance was injected at a temperature range of 228-224, 231-217 and 231-219°C, respectively. In the second test, 100, 125 and 175 µl test substance was injected at a temperature range of 229-213, 228-210 and 232-216°C, respectively. In the third test, 50, 75 and 150 µl test substance was injected at a temperature range of 230-218, 218-214 and 231-217°C, respectively.

Each test was performed using a clean test vessel.
On each day of testing, the atmospheric pressure was measured.

DATA HANDLING

The auto-ignition temperature is the lowest temperature at which the test substance will ignite when mixed with air under the conditions defined in the test method.

Deviations meet the criteria as outlined in the protocol (repeatability < 10°C when an auto-ignition temperature < 300°C is determined).

In accordance with DIN 51794, the lowest temperature at which ignition occurs in the test was rounded down to the nearest 5°C and is given as the final auto-ignition temperature.

RESULTS

Preliminary test
Starting at 20°C and testing every 20°C, a flame was observed at 240°C.
Going down from 246°C and testing every 5°C, an auto-ignition temperature of 221°C was determined.

Main study
Figure 1 shows the correlation between injected test substance volume and the auto-ignition temperature for all tests.

The auto-ignition temperature for [redacted] was 214°C (lowest determined auto-ignition temperature), with an injection volume of 125 µl and a time lag of 05 s (see Table 1).

The atmospheric pressure was 1017.0 hPa.

In conclusion, [redacted] is auto-ignitable, with an auto-ignition temperature of 210°C.

Table 1 Summary of the results of the main study

Test number	Auto-ignition Temperature [°C]	Injected volume [µl]	Time lag [s]
Test 1	228 221 223	30 70 150	02 04 03
Test 2	217 214 220	100 125 175	03 05 04
Test 3	222 218 221	50 75 150	04 05 04

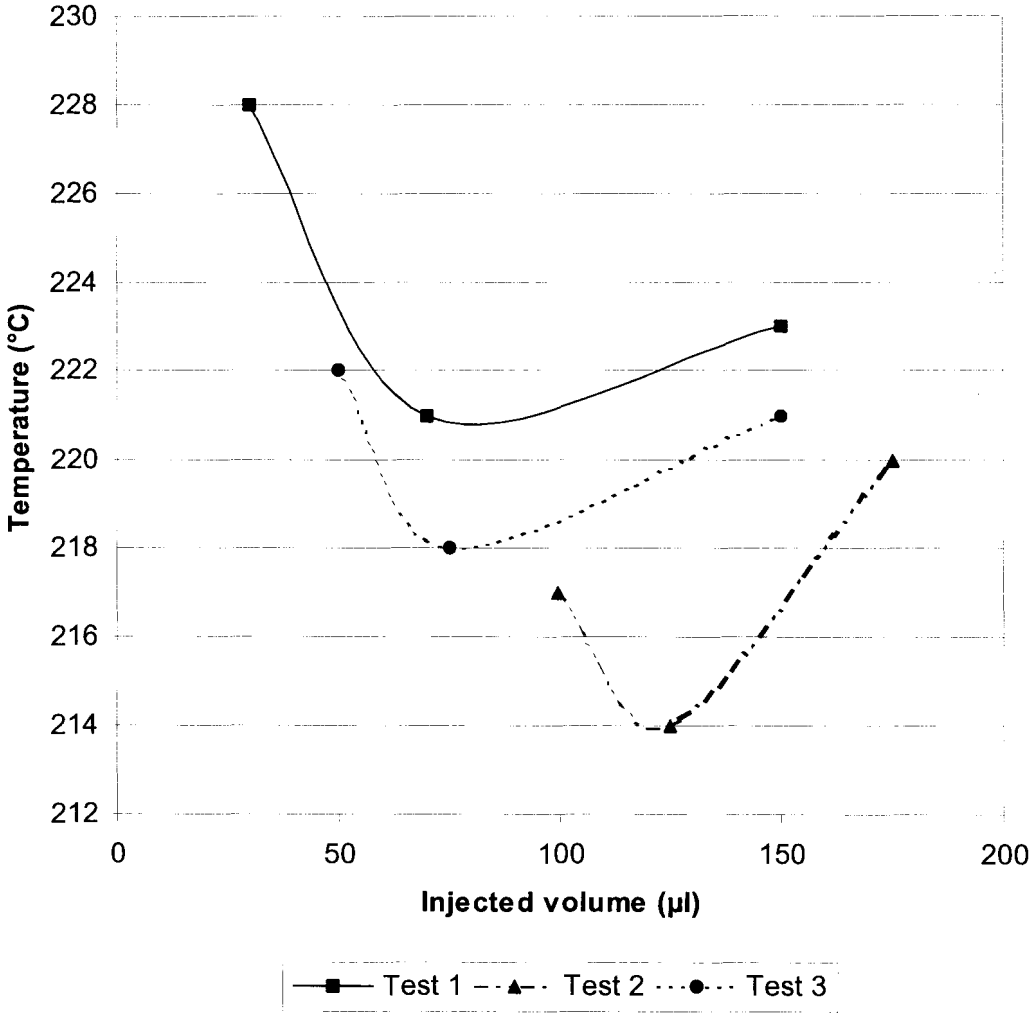

Figure 1 Correlation between auto-ignition temperature and injection volume for [redacted]

CERTIFICATE OF ANALYSIS

AKZO NOBEL

Certificate of Analysis [redacted]

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Product name : [redacted]
Chemical name : [redacted]
Batch number : **1510-14**

Test results:

Method	Analysis of	Unit	Result *[1]
Jo/72.11, [redacted]	[redacted]		
J20010792	[redacted]	% m/m	67.0 (± 1.0)
J20010792	[redacted]	% m/m	2.0 (± 0.3)
Amp/88.9	[redacted]	% m/m	2.6 (± 0.3)
J20010792	Unidentified impurities	% m/m	0.5 (± 0.2)

*[1] bracketed values are estimated 95% confidence intervals

File code : **TNA-2001007**
Analytical documentation : 20010792

Authorized by

Name [redacted]
[redacted] Section Head, Analytical Research Department
Date : October 25, 2001

Signature :

[redacted]

[redacted]

Certificate of Analysis [redacted]

[redacted]

structure	% m/m
[redacted] (Type IV) IUPAC : [redacted]	18.6
[redacted] (Type III) IUPAC : [redacted]e	7.9
[redacted]e	2.1

[redacted]s